Delocalization and the semiclassical description of molecular rotation

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We discuss phase-space delocalization for the rigid rotator within a semiclassical context by recourse to the Husimi distributions of both the linear and the $3D-$anisotropic instances. Our treatment is based upon the concomitant Fisher information measures. The pertinent Wehrl entropy is also investigated in the linear case.

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I. INTRODUCTION

We will be concerned here with the semiclassical description of the rotational dynamics of molecular systems. A pioneer effort in this sense is that of Morales *et al.* in Ref. [1], who studied the connection between such dynamics and coherent states [2, 3].

The coherent states formulation is not unique and several authors have developed alternative descriptions for molecular quantum systems. We have chosen two traditional formulations for coherent states in order to discuss the semiclassical dynamics of molecular rotational systems. One of them is devoted to two dimensional case [4] and the other to the three dimensional one [1].

In Refs. [5, 6] the authors discuss, among other things, the advantages of the Husimi distribution for the interpretation of the electronic structure in hydrogen and nitrogen atoms. They suggested that their work may be extended to the molecular instance. Following this suggestion we address here the simplest applicable model, i.e., the rigid rotator. Its usefulness for describing diatomic molecules is well-known [7].

Delocalization is an "energetically favorable" process, since it distributes the wave of function over a volume greater than the size of the sample. Thus, the net energy of the molecule is lowered, which results in resonance-stabilization. The celebrated Fisher information $\mathcal{I}$ [8, 9, 10, 13] can be related to the delocalization measure as follows: if we take a wave package with a standard deviation σ the Fisher information is given by $\mathcal{I} \geq 1/\sigma^2$, thus, in this sense, we realize that the Fisher information is a quite sensitive indicator of the delocalization of the wave package [8, 9, 10].

The rigid rotator is a system of a single particle whose quantum spectrum of energy is exactly known. Therefore, the study of typical thermodynamic properties can be analytically derived[11]. Applications lead to the treatment of important aspects of molecular systems[12]. The paper is organized as follows: In Section II we explore the linear rigid rotator. We write the probability of finding a quantum state in a coherent state that is used to obtain an explicit expression for the (i) Husimi distribution, (ii) Wehrl entropy, and (iii) Fisher Information. These results are of help in Section III, where we discuss a model for the three dimensional rigid rotator. Finally, in Section IV, we draw some conclusions.

II. LINEAR RIGID ROTATOR

We start the present study by exploring a simple model, the linear rigid rotator (LRR), based on the excellent discussion concerning the coherent states for angular momenta given in Ref. [14]. The LRR-hamiltonian writes [7]

$$\hat{H} = \frac{\hat{L}^2}{2I_{xy}}, \tag{1}$$

where $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2$ is the angular momentum operator and I_x and I_y are the associated moments of inertia. We have assumed that $I_{xy} \equiv I_x = I_y$. Calling $|I, K\rangle$ the set of H-eigenstates, we recall that they verify the relations

$$\begin{aligned} \hat{L}^2|IK\rangle &= I(I+1)|IK\rangle \\ \hat{L}_z|IK\rangle &= K|IK\rangle, \end{aligned} \tag{2}$$

with $I = 0, 1, 2\ldots$, for $-I \leq K \leq I$, the eigenstates'

energy spectrum being given by

$$\varepsilon_I = \frac{I(I+1)\hbar^2}{2I_{xy}}, \tag{3}$$

where for simplicity we take $\hbar = 1$.
We construct the lineal coherent states for the rigid rotator using Schwinger's oscillator model of angular momentum [4, 15] as

$$|IK\rangle = \frac{(\hat{a}_+^\dagger)^{I+K}(\hat{a}_-^\dagger)^{I-K}}{\sqrt{(I+K)!(I-K)!}}|0\rangle, \tag{4}$$

with $\hat{a}_+$ and $\hat{a}_-$ the pertinent creation and annihilation operators, respectively, and $|0\rangle \equiv |0,0\rangle$ the vacuum state. The states $|IK\rangle$ are orthogonal and satisfy the closure relation, i.e.,

$$\langle I^{'}K^{'}|IK\rangle = \delta_{I',I}\delta_{K',K}, \tag{5}$$

$$\sum_{I=0}^{\infty}\sum_{K=-I}^{I}|IK\rangle\langle IK| = \hat{1}. \tag{6}$$

Since we deal with two degrees of freedom the ensuing coherent states are of the tensorial product form (involving $|z_1\rangle$ and $|z_2\rangle$) [14]

$$|z_1z_2\rangle = |z_1\rangle \otimes |z_2\rangle, \tag{7}$$

where

$$\hat{a}_+|z_1z_2\rangle = z_1|z_1z_2\rangle, \tag{8}$$

$$\hat{a}_-|z_1z_2\rangle = z_2|z_1z_2\rangle. \tag{9}$$

Therefore, the coherent state $|z_1z_2\rangle$ writes [14]

$$|z_1z_2\rangle = e^{-\frac{|z|^2}{2}}e^{z_1\hat{a}_+^\dagger}e^{z_2\hat{a}_-^\dagger}|0\rangle, \tag{10}$$

with

$$\begin{aligned} |z_1\rangle &= e^{-\frac{|z_1|^2}{2}}\,e^{z_1\hat{a}_+^\dagger}|0\rangle, & (11)\\ |z_2\rangle &= e^{-\frac{|z_2|^2}{2}}\,e^{z_2\hat{a}_-^\dagger}|0\rangle. & (12)\end{aligned}$$

We have introduced the convenient notation

$$|z|^2 = |z_1|^2 + |z_2|^2. \tag{13}$$

Using Eqs. (4) and (10) we easily calculate $\langle IK|z_1z_2\rangle$ and, after a bit of algebra, find

$$\langle IK|z_1z_2\rangle = e^{-\frac{|z|^2}{2}}\,\frac{z_1^{n_+}}{\sqrt{n_+!}}\,\frac{z_2^{n_-}}{\sqrt{n_-!}} \tag{14}$$

where $n_+ = I+K$ and $n_- = I-K$. Therefore, the probability of observing the state $|IK\rangle$ in the coherent state $|z_1z_2\rangle$ is of the form

$$|\langle IK|z_1z_2\rangle|^2 = e^{-|z|^2}\,\frac{z_1^{2n_+}}{n_+!}\,\frac{z_2^{2n_-}}{n_-!}. \tag{15}$$

A. Husimi distribution

Following the procedure developed by Anderson *et al.* [16], we can readily calculate the Husimi distribution [17], which is defined as

$$\mu(z_1,z_2) = \langle z_1,z_2|\hat{\rho}|z_1,z_2\rangle, \tag{16}$$

where the density operator is

$$\hat{\rho} = Z_{2D}^{-1}\exp{(-\beta\hat{\mathcal{H}})}, \tag{17}$$

and $\beta = 1/k_BT$, k_B is the Boltzmann's constant and T the temperature. The form of the rotational partition function Z_{2D} is given in Ref. [7]

$$Z_{2D} = \sum_{I=0}^{\infty}(2I+1)\,e^{-I(I+1)\frac{\Theta}{T}}, \tag{18}$$

with $\Theta = \hbar^2/(2I_{xy}k_B)$. In the present context, speaking of the "trace operation" entails performing the sum $\mathrm{Tr} \equiv \sum_{I=0}^{\infty}\sum_{K=-I}^{I}$.
Inserting the closure relation into Eq. (16), and using Eq. (15), we finally get our Husimi distributions in the fahion

$$\mu(z_1,z_2) = e^{-|z|^2}\,\frac{\sum_{I=0}^{\infty}\frac{|z|^{4I}}{(2I)!}\,e^{-I(I+1)\,\frac{\Theta}{T}}}{\sum_{I=0}^{\infty}(2I+1)\,e^{-I(I+1)\frac{\Theta}{T}}}. \tag{19}$$

It is easy to show that this distribution is normalized to unity

$$\int\frac{\mathrm{d}^2z_1}{\pi}\frac{\mathrm{d}^2z_2}{\pi}\,\mu(z_1,z_2) = 1, \tag{20}$$

where z_1 and z_2 are given by Eqs. (8), (9), and (13). Note that we must deal with the binomial expression $(|z_1|^2+|z_2|^2)^{4I}$ firstly and then integrate over the whole complex plane (in two dimensions) in order to verify the normalization condition (20). The differential element of area in the $z_1(z_2)$ plane is $\mathrm{d}^2z_1 = \mathrm{d}x\mathrm{d}p_x/2\hbar$ ($\mathrm{d}^2z_2 = \mathrm{d}y\mathrm{d}p_y/2\hbar$) [2]. Moreover, we have the phase-space relationships

$$|z_1|^2 = \frac{1}{4}\left(\frac{x^2}{\sigma_x^2}+\frac{p_x^2}{\sigma_{p_x}^2}\right), \tag{21a}$$

$$|z_2|^2 = \frac{1}{4}\left(\frac{y^2}{\sigma_y^2} + \frac{p_y^2}{\sigma_{p_y}^2}\right), \tag{21b}$$

where $\sigma_x \equiv \sigma_y = \sqrt{\hbar/2m\omega}$ and $\sigma_{p_x} \equiv \sigma_{p_y} = \sqrt{\hbar m\omega/2}$. In Fig. 1, we depict the behavior of the Husimi distribution $\mu(z_1, z_2)$ as a function of $|z|$ at fixed temperature. The profile of the Husimi function is similar to Gaussian distribution.

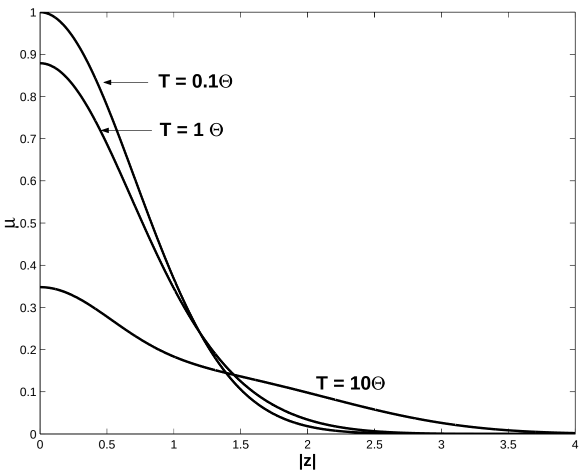

FIG. 1: It is depicted the Husimi function $\mu(z_1, z_2)$ as a function of $|z|$ for several values of the temperature, ($T = 0.1\Theta, \Theta, 10\Theta$) for the linear rotator. The behavior of the Husimi function looks like Gaussian distribution. The peak of the distribution increases as the temperature decreases.

B. Wehrl entropy and Fisher Information

The Wehrl entropy is a semiclassical measure of localization [18]. So is Fisher's one [13]. The Wehrl measure is simply a logarithmic Shannon measure built up with Husimi distributions. For the present bi-dimensional model this entropy is of the form

$$\mathcal{W} = \int \frac{\mathrm{d}^2 z_1}{\pi}\frac{\mathrm{d}^2 z_2}{\pi}\, \mu(z_1, z_2)\, \ln \mu(z_1, z_2), \tag{22}$$

where $\mu(z_1, z_2)$ is given by Eq. (19). The so-called phase-space, shift-invariant Fisher measure [13] is a particular instance of the general Fisher-one [9, 10], that can be regarded as an (also semiclassical) counterpart of Wehrl entropy [13]. Extending now to the present $2D-$case the ideas developed in Ref. [13] for the case of the $1D-$harmonic oscillator, we define the (phase-space) shift invariant Fisher measure in the fashion

$$\mathcal{I} = \int \frac{\mathrm{d}^2 z_1}{\pi}\frac{\mathrm{d}^2 z_2}{\pi}\, \mu(z_1, z_2)\, \mathcal{A}, \tag{23}$$

with

$$\mathcal{A} = \sum_{\Lambda=\{x,p_x,y,p_y\}} \sigma_\Lambda^2 \left[\frac{\partial \ln \mu(z_1, z_2)}{\partial \Lambda}\right]^2, \tag{24}$$

where we have introduced a simplified in which the index Λ successively takes the values x, p_x, y, and p_y, respectively. It is easy to prove that the quantity $\mathcal{A}$ has the following form –see details in appendix V–

$$\mathcal{A} = \eta(z_1, z_2)^2, \tag{25}$$

where

$$\eta(z_1, z_2) = \frac{\sum_{I=0}^{\infty}\left[\frac{|z|^{4I-1}}{(2I-1)!} - \frac{|z|^{4I+1}}{(2I)!}\right] e^{-I(I+1)\Theta/T}}{\sum_{I=0}^{\infty}\frac{|z|^{4I}}{(2I)!}\, e^{-I(I+1)\Theta/T}}. \tag{26}$$

Therefore, the corresponding Fisher measure acquires the simpler appearance

$$\mathcal{I} = \int \frac{\mathrm{d}^2 z_1}{\pi}\frac{\mathrm{d}^2 z_2}{\pi}\, \mu(z_1, z_2)\ \eta(z_1, z_2)^2, \tag{27}$$

i.e.,

$$\mathcal{I} \equiv \langle \eta(z_1, z_2)^2 \rangle, \tag{28}$$

where with the notation

$$\langle \mathcal{G} \rangle = \int \frac{\mathrm{d}^2 z_1}{\pi}\frac{\mathrm{d}^2 z_2}{\pi}\, \mu(z)\, \mathcal{G}, \tag{29}$$

we allude to the *semi-classical expectation value* of $\mathcal{G}$. In Fig. 2 we plot both Fisher's information and Wehrl's entropy as a function of T/Θ. They behave in different manner. If the temperature $T \to 0$, Fisher's information measure (inverse-delocalization) takes its maximum value and Wehrl's its minimum. This behavior is reversed for high temperatures, with the degree of delocalization becoming larger and larger.

III. RIGID ROTATOR IN THREE DIMENSIONS

In the present section we consider a more general problem, the $3D-$rigid rotator model, whose hamiltonian writes [1]

$$\hat{H} = \frac{\hat{L}_x^2}{2I_x} + \frac{\hat{L}_y^2}{2I_y} + \frac{\hat{L}_z^2}{2I_z}, \tag{30}$$

where I_x, I_y, and I_z are the associated moments of inertia. A complete set of rotor eigenstates is $\{|IMK\rangle\}$. The following relations apply

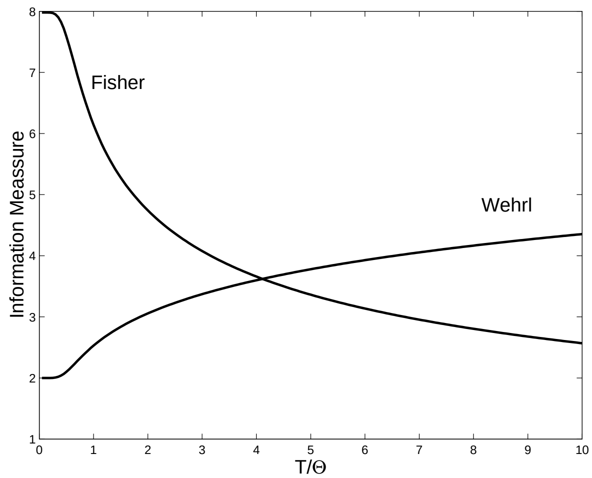

FIG. 2: The trend of the Fisher information measure (delocalization) ($\mathcal{I}$) in comparison with the Wehrl entropy ($\mathcal{W}$) as a function of the temperature are shown for the linear rotator. We see that, if the temperature increases, then the delocalization decreases while Wehrl entropy increases.

$$\begin{aligned} \hat{L}^2|IMK\rangle &= I(I+1)|IMK\rangle \\ \hat{L}_z|IMK\rangle &= K|IMK\rangle \\ \hat{J}_z|IMK\rangle &= M|IMK\rangle, \end{aligned} \tag{31}$$

where $I = 0, \ldots, \infty, -I \leq K \leq I$, and $-I \leq M \leq I$. The states $|IMK\rangle$ satisfy orthogonality and closure relations [1]

$$\langle I^{'}M^{'}K^{'}|IMK\rangle = \delta_{I^{'},I}\delta_{M^{'},M}\delta_{K^{'},K} \tag{32}$$

$$\sum_{I=0}^{\infty}\sum_{M=-I}^{I}\sum_{K=-I}^{I}|IMK\rangle\langle IMK| = \hat{1}. \tag{33}$$

If we take $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ and assume axial symmetry, i.e., $I_{xy} \equiv I_x = I_y$, we can recast the hamiltonian as

$$\hat{H} = \frac{1}{2I_{xy}}\left[\hat{L}^2 + \left(\frac{I_{xy}}{I_z} - 1\right)\hat{L}_z^2\right], \tag{34}$$

where $\hat{L}^2$ is the angular momentum operator and $\hat{L}_z$ is its projection on the rotation axis z. The concomitant spectrum of energy becomes

$$\varepsilon_{I,K} = \frac{\hbar^2}{2I_{xy}}\left[I(I+1) + \left(\frac{I_{xy}}{I_z} - 1\right)K^2\right], \tag{35}$$

where $I = 0, 1, 2, \cdots$ and it represents the eigenvalue of the angular momentum operator $\hat{L}^2$, the numbers $m = -I, \cdot\cdot\cdot, -1, 0, 1, \cdot\cdot\cdot, I$ represent the projections on the intrinsic rotation axis of the rotor. All states present a degeneracy given by $(2I+1)$. The parameters $I_x = I_y \equiv I_{xy}$ and I_z are the inertia momenta. Several geometrical cases are characterized through the I_{xy}/I_z ratio. For instance, the marginal value $I_{xy}/I_z = 1$ corresponds to the spherical rotor. Limiting cases can be considered; this is, $I_{xy}/I_z = 1/2$ and $I_{xy}/I_z \to \infty$ that correspond to the extremely oblate and prolate cases, respectively.

A. Coherent states

In order to obtain the Husimi distribution for this problem we need first of all to construct the associated coherent states, as already discussed by Morales *et al.* in Ref. [1]. Introduce first the auxiliary quantity

$$X_{I,M,K} = \sqrt{I!(I+M)!(I-M)!(I+K)!(I-K)!}, \tag{36}$$

and then write [1]

$$|z_1z_2z_3\rangle = e^{-\frac{|u|^2}{2}}\sum_{IMK}\frac{[(2I)!]^2 z_1^{(I+M)} z_2^I z_3^{(I+K)}}{X_{I,M,K}}|IMK\rangle, \tag{37}$$

where the following supplementary variable were introduced [1]

$$|u|^2 = |z_2|^2(1+|z_1|^2)^2(1+|z_3|^2)^2. \tag{38}$$

B. Husimi function, Wehrl entropy, and Fisher measure

Using now Eq. (37) we find

$$|\langle IMK|z_1z_2z_3\rangle|^2 = \frac{e^{-|u|^2}}{X_{I,M,K}^2}[(2I)!]^2|z_1|^{2(I+M)}|z_2|^{2I}|z_3|^{2(I+K)} \tag{39}$$

and determine that, in this case, the rotational partition function reads

$$Z_{3D} = \sum_{I=0}^{\infty}\sum_{K=-I}^{I}\sum_{M=-I}^{I}e^{-\beta\varepsilon_{I,K}}, \tag{40}$$

i.e.,

$$Z_{3D} = \sum_{I=0}^{\infty}(2I+1)\,e^{-I(I+1)\frac{\Theta}{T}}\sum_{K=-I}^{I}e^{-\left(\frac{I_{xy}}{I_z}-1\right)K^2\frac{\Theta}{T}}. \tag{41}$$

It is convenient to remark that if we take one of limiting cases, this the extremely prolate, $I_{xy}/I_z \to \infty$, the only term that survives in the right sum of the right side in Eq.(41) is that for $K = 0$ and all terms for $K \neq 0$ vanish; in such particular case Z_{2D} is recovered from Z_{3D}.

The pertinent Husimi distribution then becomes

$$\mu(z_1,z_2,z_3)=\frac{e^{-|u|^2}}{Z_{3D}}\sum_{I=0}^{\infty}\frac{(2I)!}{I!}\,|v|^{2I}\,e^{-I(I+1)\frac{\Theta}{T}}\times g(I) \tag{42}$$

where

$$g(I)=\sum_{K=-I}^{I}\frac{|z_3|^{2(I+K)}}{(I+K)!(I-K)!}\,e^{-\left(\frac{I_{xy}}{I_z}-1\right)K^2\frac{\Theta}{T}}, \tag{43}$$

with

$$|v|^2=(1+|z_1|^2)^2|z_2|^2, \tag{44a}$$

$$|u|^2=|v|^2(1+|z_3|^2)^2. \tag{44b}$$

We can easily verify that $\mu(z_1,z_2,z_3)$ is normalized in the fashion

$$\int \mathrm{d}\Gamma\,\mu(z_1,z_2,z_3)=1, \tag{45}$$

where $\mathrm{d}\Gamma$ is the measure of integration given by [1]

$$\begin{aligned}\mathrm{d}\Gamma \;=\; \mathrm{d}\tau\Big\{&4[(1+|z_1|^2)(1+|z_3|^2)]^4|z_2|^4-\\ &-8[(1+|z_1|^2)(1+|z_3|^2)]^2|z_2|^2+1\Big\}\end{aligned} \tag{46}$$

with

$$\mathrm{d}\tau=\frac{\mathrm{d}^2z_1}{\pi}\frac{\mathrm{d}^2z_2}{\pi}\frac{\mathrm{d}^2z_3}{\pi}, \tag{47}$$

where, of course, in this case we have three degrees of freedom.

We compute then, the Wherl entropy in the form

$$\mathcal{W}=\int \mathrm{d}\Gamma\,\mu(z_1,z_2,z_3)\,\ln\mu(z_1,z_2,z_3), \tag{48}$$

and explicitly the Fisher measure as follows

$$\mathcal{I}=\int \mathrm{d}\Gamma\,\mu(z_1,z_2,z_3)\,\mathcal{A}_{3D} \tag{49}$$

where in this case we define the quantity $\mathcal{A}_{3D}$ in three dimensions as

$$\mathcal{A}_{3D}=\sum_{\Lambda=\{x,p_x,y,p_y,z,p_z\}}\sigma_\Lambda^2\left[\frac{\partial\ln\mu(z_1,z_2,z_3)}{\partial\Lambda}\right]^2, \tag{50}$$

with the phase space relationships (21a), (21b) and

$$|z_3|^2=\frac{1}{4}\left(\frac{z^2}{\sigma_z^2}+\frac{p_z^2}{\sigma_{p_z}^2}\right), \tag{51}$$

where $\sigma_z=\sqrt{\hbar/2m\omega}$ and $\sigma_{p_z}=\sqrt{\hbar m\omega/2}$. In this instance $\mathrm{d}^2z_3=\mathrm{d}z\mathrm{d}p_z/2\hbar$. So, after a bit of algebra we arrive to

$$\begin{aligned}\mathcal{I} \;=\; &\int \mathrm{d}\Gamma\,\mu(z_1,z_2,z_3)\Big\{\gamma^2(|z_1|^2|z_2|^2+\frac{1}{4}(1+|z_1|^2)^2)+\\ &+4|u|^2|z_3|^2\Big\},\end{aligned} \tag{52}$$

i.e.,

$$\mathcal{I}=\langle\gamma^2(|z_1|^2|z_2|^2+\frac{1}{4}(1+|z_1|^2)^2)+4|u|^2|z_3|^2\rangle \tag{53}$$

where

$$\begin{aligned}\gamma \;=\; &\frac{-(1+|z_3|^2)^2\sum_{I=0}^{\infty}\frac{2(2I)!}{I!}\,|v|^{2I+1}\,e^{-I(I+1)\frac{\Theta}{T}}\times g(I)}{\sum_{I=0}^{\infty}\frac{(2I)!}{I!}\,|v|^{2I}\,e^{-I(I+1)\frac{\Theta}{T}}\times g(I)}+\\ &+\frac{\sum_{I=0}^{\infty}\frac{2(2I)!}{(I-1)!}\,|v|^{2I-1}\,e^{-I(I+1)\frac{\Theta}{T}}\times g(I)}{\sum_{I=0}^{\infty}\frac{(2I)!}{I!}\,|v|^{2I}\,e^{-I(I+1)\frac{\Theta}{T}}\times g(I)}.\end{aligned} \tag{54}$$

In the special instance $I_{xy}/I_z=1$, that corresponds to the spherical rotor, we can explicitly obtain

$$\mu(z_1,z_2,z_3)=e^{-|u|^2}\,\frac{\sum_{I=0}^{\infty}\frac{|u|^{2I}}{I!}\,e^{-I(I+1)\frac{\Theta}{T}}}{\sum_{I=0}^{\infty}(2I+1)^2\,e^{-I(I+1)\frac{\Theta}{T}}}. \tag{55}$$

Having the Husimi functions the Wehrl entropy is straightforwardly computed.

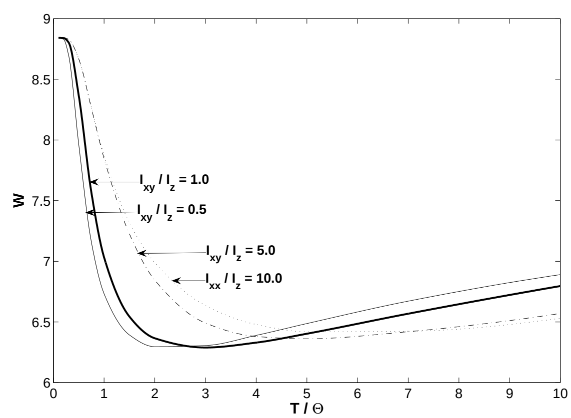

FIG. 3: A family of Wehrl entropy $\mathcal{W}$ as a function of T/Θ is depicted for the 3D anisotropic rigid rotator for several values of the anisotropy ($I_{xy}/I_z=1/2,1,5,10$). The trend of the Wehrl entropy is not very similar to the linear case, it has a maximum in $T/\Theta=0$, a minimum in $T/\Theta\geq 2$, whose exact value depends on the ratio I_{xy}/I_z.

In figure 3 we compare the Wehrl entropy $\mathcal{W}$, as a function of T/Θ, for several values of I_{xy}/I_z; this is, the

extremely oblate rotator $I_{xy}/I_z = 1/2$ (e.g., $CHCl_3$ and C_6H_6), the prolate rotator $I_{xy}/I_z = 5, 10$ (e.g., CH_3Cl and PCl_5) and the spherical case $I_{xy}/I_z = 1$. Unfortunately, from the 3D formulation of coherent states is not possible to recover the form of the Wehrl entropy, in the same way as occurs with the partition function from the Eq.(41), which is conveniently lead to the form of the Eq.(18) in the limiting case of the extremely prolate rotator $I_{xy}/I_z \to \infty$. It could be due to a note given in Ref.[1], the present version of coherent states formulation is weak because the measure from the Eq.(46) is not positive.

IV. CONCLUDING REMARKS

We have concentrated our effort on the study of the semi-classical behavior of the rigid rotator and have obtained in analytical fashion the form of the Husimi distribution for two cases, namely, the linear and the axially symmetric rigid rotator. As it is expected, the linear case is obtained as a particular case from the formulation in three dimensions. Also, we have obtained an analytical expression of the shift-invariant Fisher measure built up with Husimi distribution, for the rigid rotator model, concluding that Fisher measure is better indicator of the delocalization than Wherl entropy for this model. The present study could motivate other specialists to improve the present formulation of the coherent states in order to recover all quantities in two dimensions from a formulation in three dimensions.

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V. APPENDIX: A BIT OF ALGEBRA

First of all, we carry out the differentiation the Husimi distribution (19) with respect to the variable x, obtaining the following result

$$\frac{\partial \ln \mu(z_1, z_2)}{\partial x} = 2\eta(z_1, z_2)\frac{\partial |z|}{\partial x} \tag{56}$$

where the quantity $\eta(z_1, z_2)$ was defined in Eq. (26). Moreover, from Eqs. (21a) and (21b) we have

$$\frac{\partial |z|}{\partial x} = \frac{x}{4|z|\sigma_x^2}, \tag{57}$$

and we are lead to

$$\frac{\partial \ln \mu(z_1, z_2)}{\partial x} = \frac{\eta(z_1, z_2)x}{2|z|\sigma_x^2}. \tag{58}$$

We arrive to a similar expression differentiating with respect to p_x,

$$\frac{\partial \ln \mu(z_1, z_2)}{\partial p_x} = \frac{\eta(z_1, z_2)p_x}{2|z|\sigma_{p_x}^2}. \tag{59}$$

Analogous expressions are obtained replacing x and p_x for y and p_y. Finally, substituting these results into Eq. (24) we thus arrive to

$$\mathcal{A} = \eta(z_1, z_2)^2. \tag{60}$$